The Green Lab Notebook:

Chemical intelligence and green informatics in a mobile app

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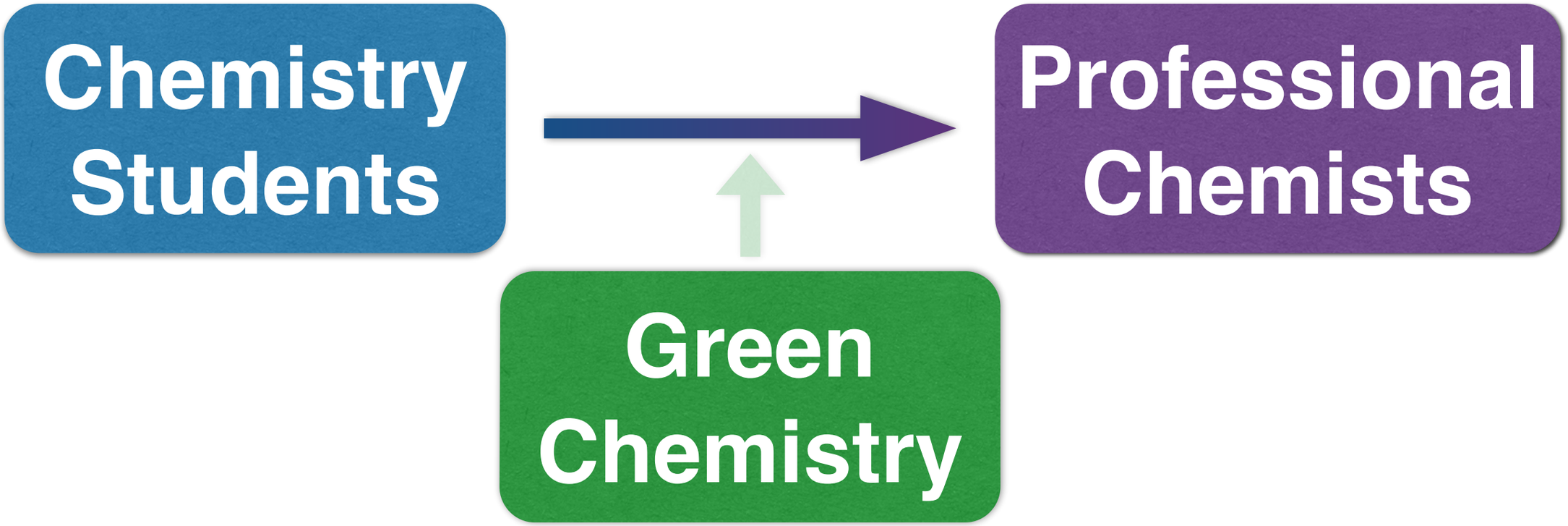
http://molmatinf.com



- **Green chemistry** is like a distinct profession:
  - its own journals, grants, conferences…
- **Students** need to develop habits early
- **Professionals** need information access

Software Can Help

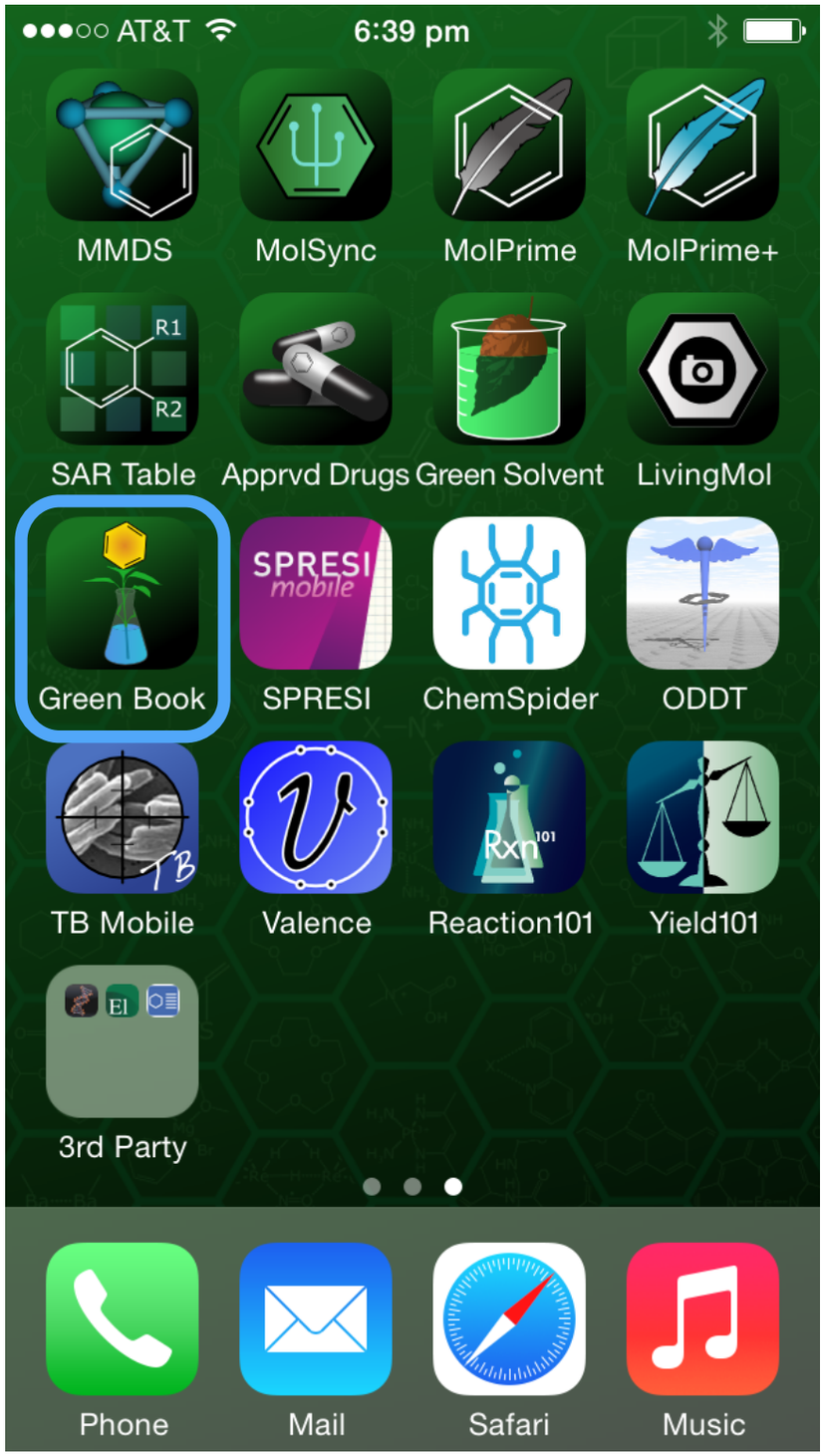
Calculations

- percentage yield
- atom efficiency
- process mass intensity
- E-factor

Information

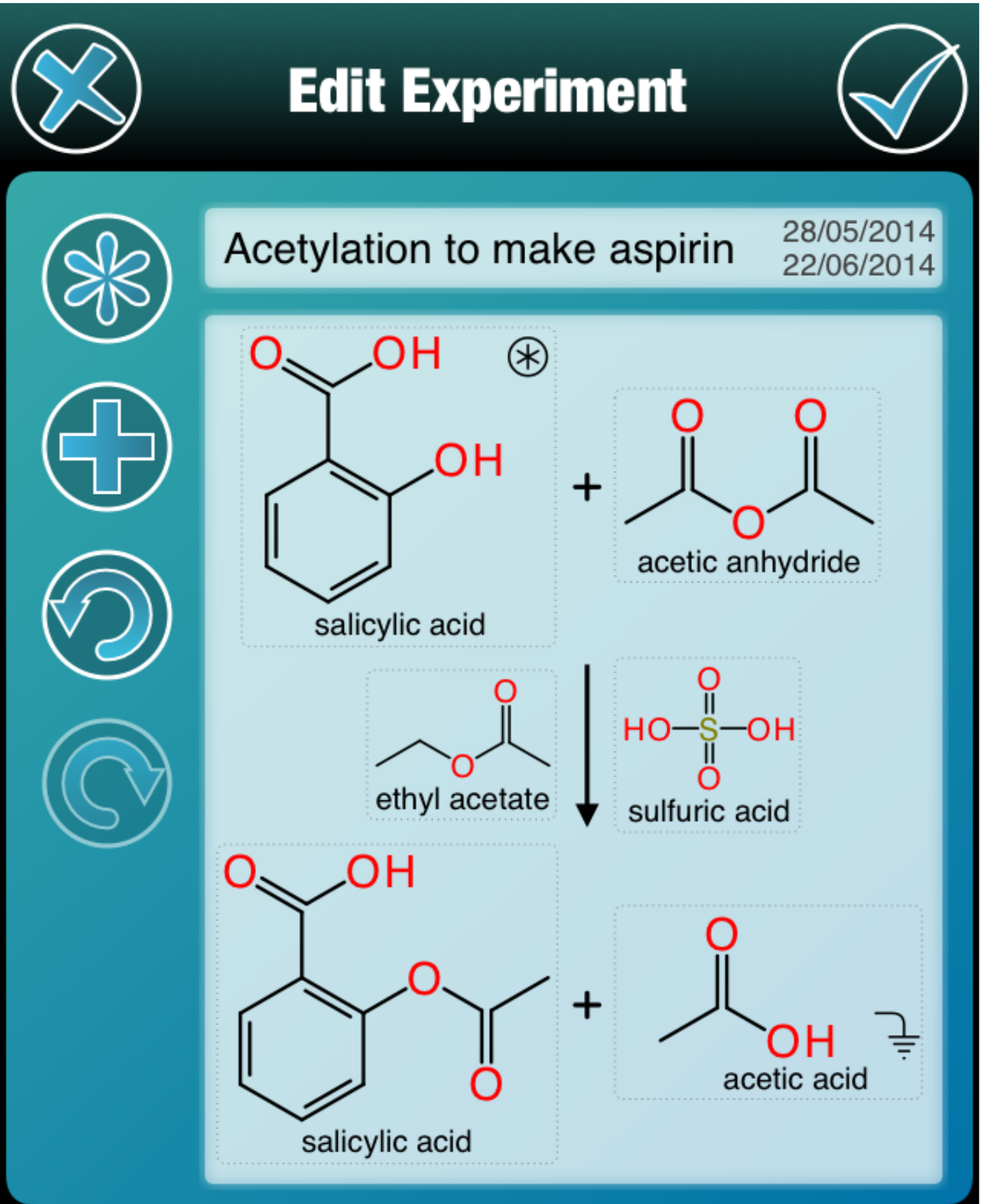
- greener solvents
- sustainable feedstocks
- hazardous byproducts
- benign reactions

Mobile App



- Mobile: the platform of the future
- Where the action is: UX/UI innovation
- Where the students are now: iPhones, iPads, etc.
- Needs to be accessible, affordable, simple, effective…

Making Aspirin



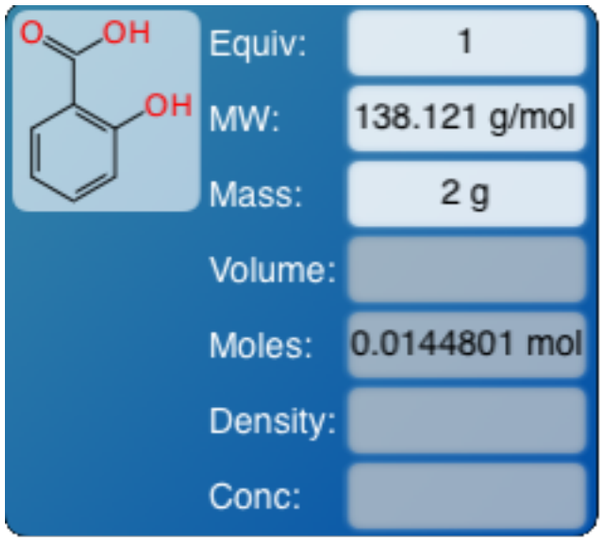
- The quintessential undergraduate reaction…

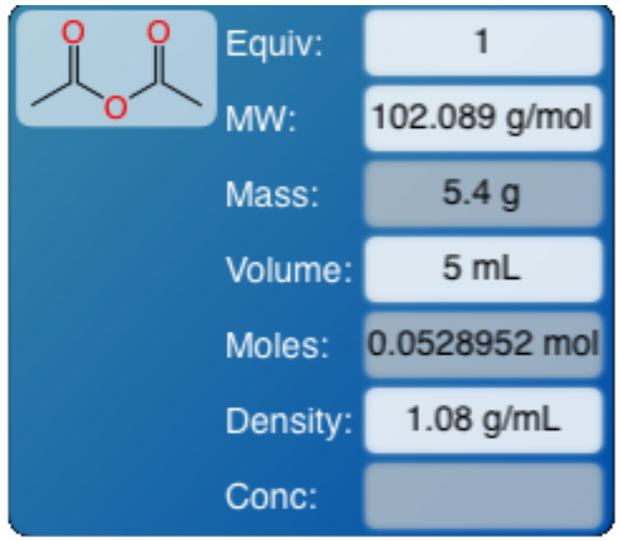
Reactants

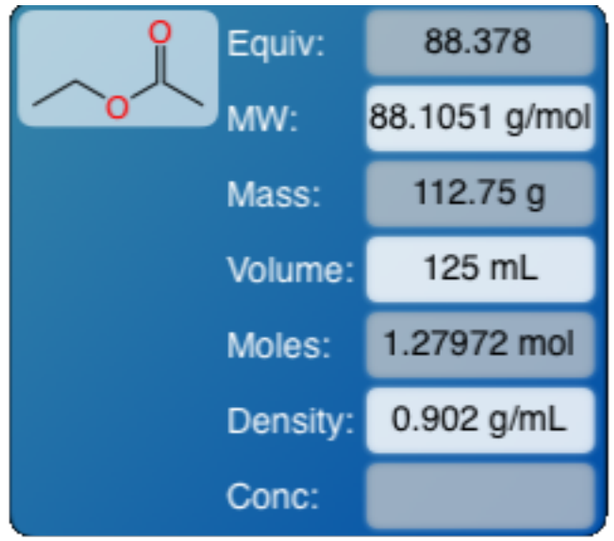
Reagents

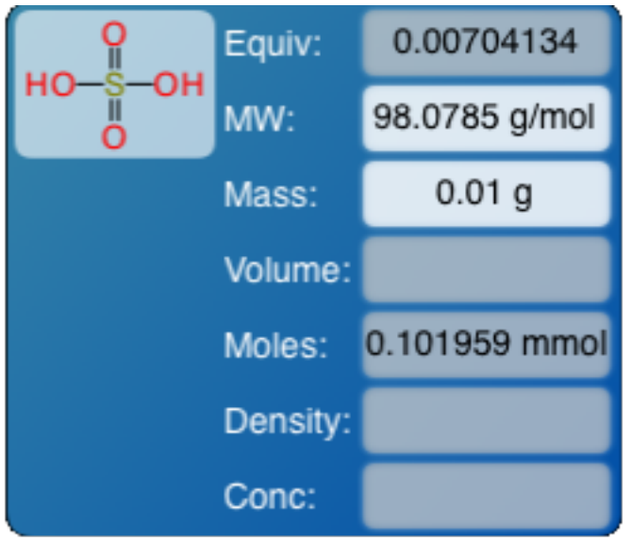
Products

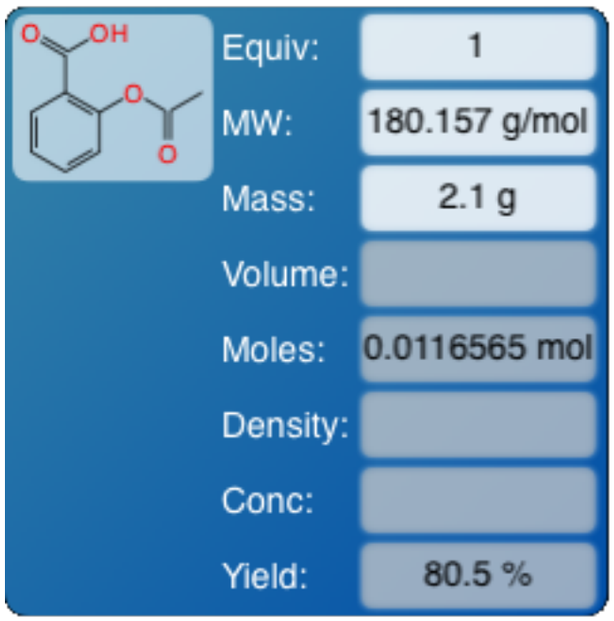
Entering Quantities

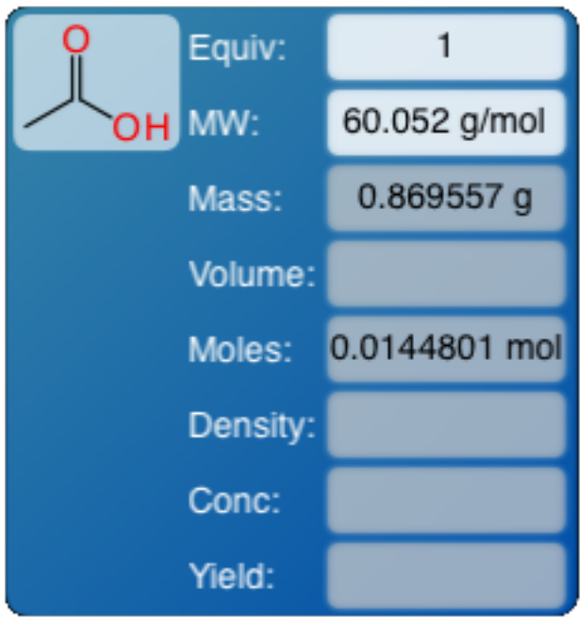












- Use the app to enter quantities for each reaction component

- Automagic calculation of **molecular weight**, **moles**, **volume** ↔ **mass** (*density*, *concentration*), **yield**

Calculations

Yield

$$\frac{\text{actual product amount}}{\text{theoretical product amount}}$$

☞ 100%

Atom Economy

$$\frac{\sum \text{product molecular weight}}{\sum \text{reactant molecular weight}}$$

☞ 100%

Process Mass Intensity

$$\frac{\sum \text{reactant mass}}{\sum \text{product mass}}$$

☞ 1

E-factor

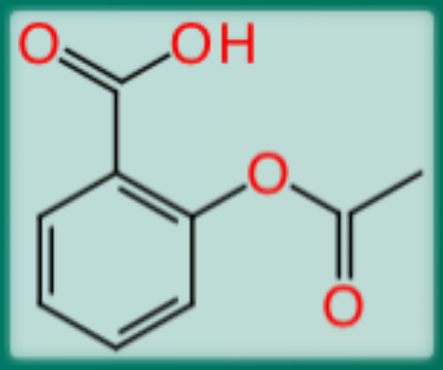
$$\frac{\sum \text{waste mass}}{\sum \text{product mass}}$$

☞ 0

Automatic Green Metrics

- Green metrics are *always calculated…*

Σ reactants = 2 g + 5.4 g + 112.75 g + 0.01 g = 120.16 g **Σ products** = 2.1 g = 2.1 g **Σ waste** = 0.869557 g = 0.869557 g



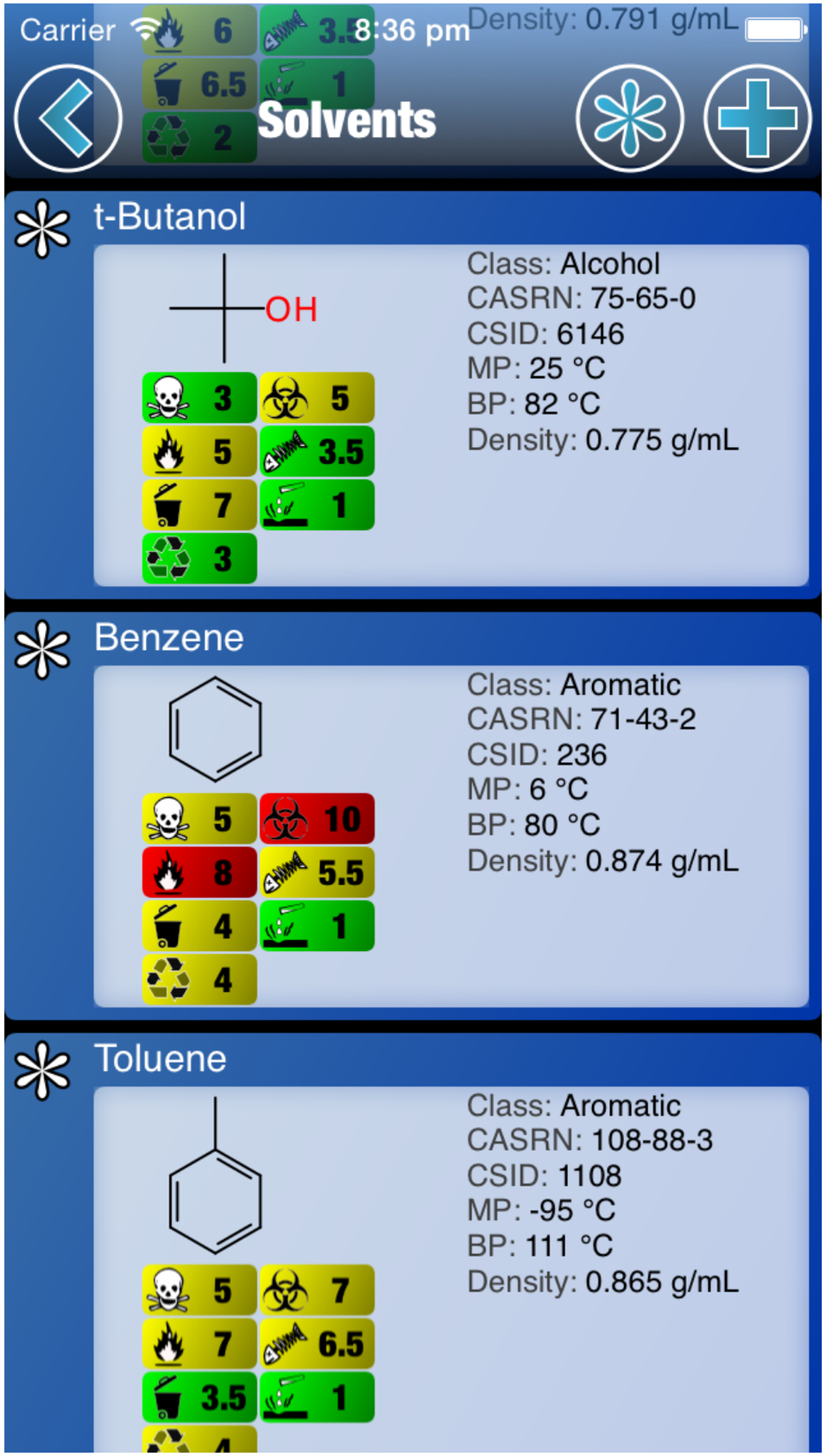
$$\text{PMI} = \frac{2\text{ g} + 5.4\text{ g} + 112.75\text{ g} + 0.01\text{ g}}{2.1\text{ g}} = 57.2191$$

$$\text{E-factor} = \frac{0.869557\text{ g} + 117.19\text{ g}}{2.1\text{ g}} = 56.2191$$

$$\text{Atom-E} = \frac{180.157}{138.121 + 102.089} = 75.0002\ \%$$

- … always shown, always stored
- These metrics become as accessible as yield
- Easier to compare & optimise for greenness

Solvents



- Choice of solvent has a huge impact on green profile

- Curated data regarding:

Safety

Health

Flammability

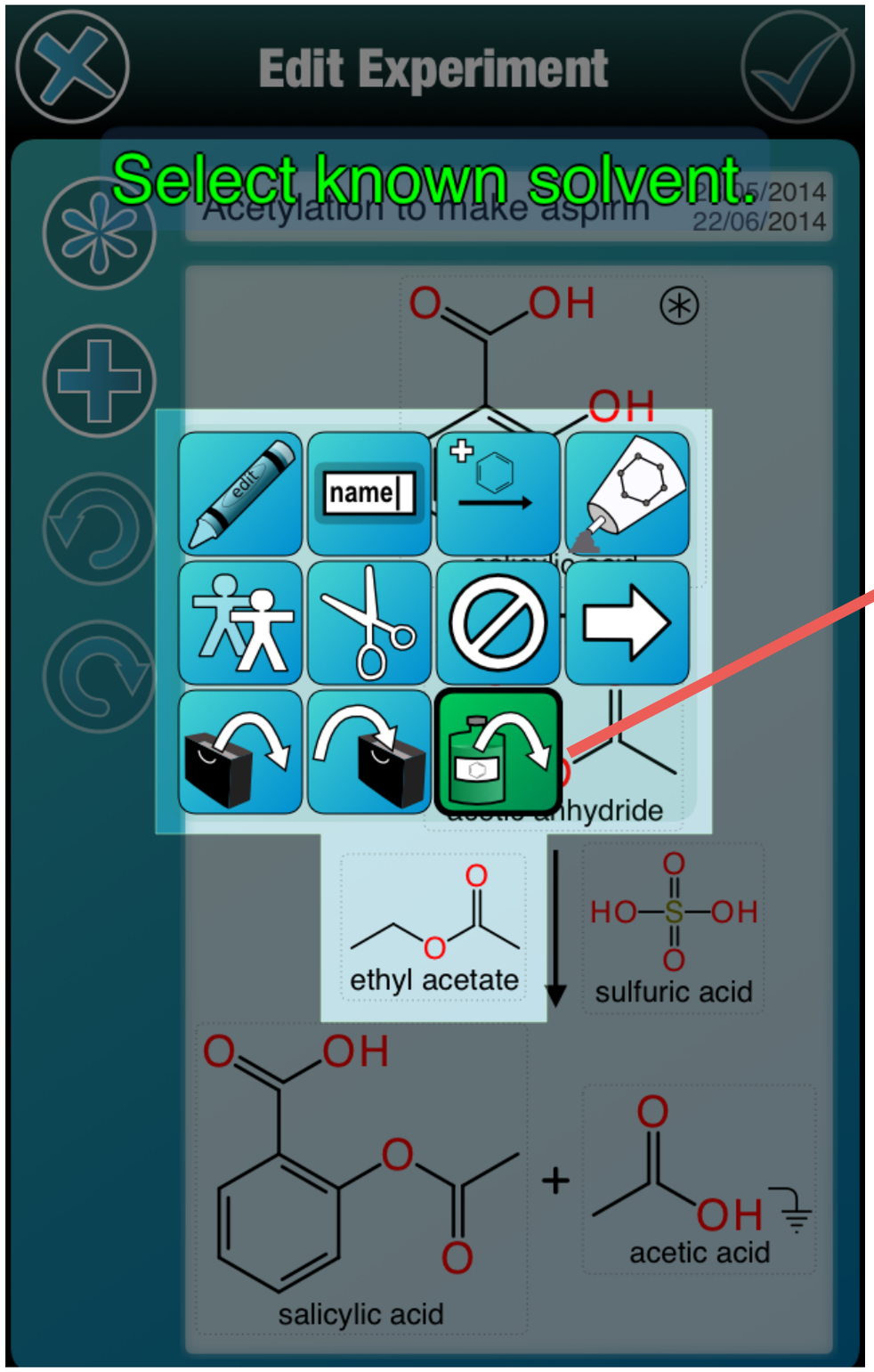
Environmental impact

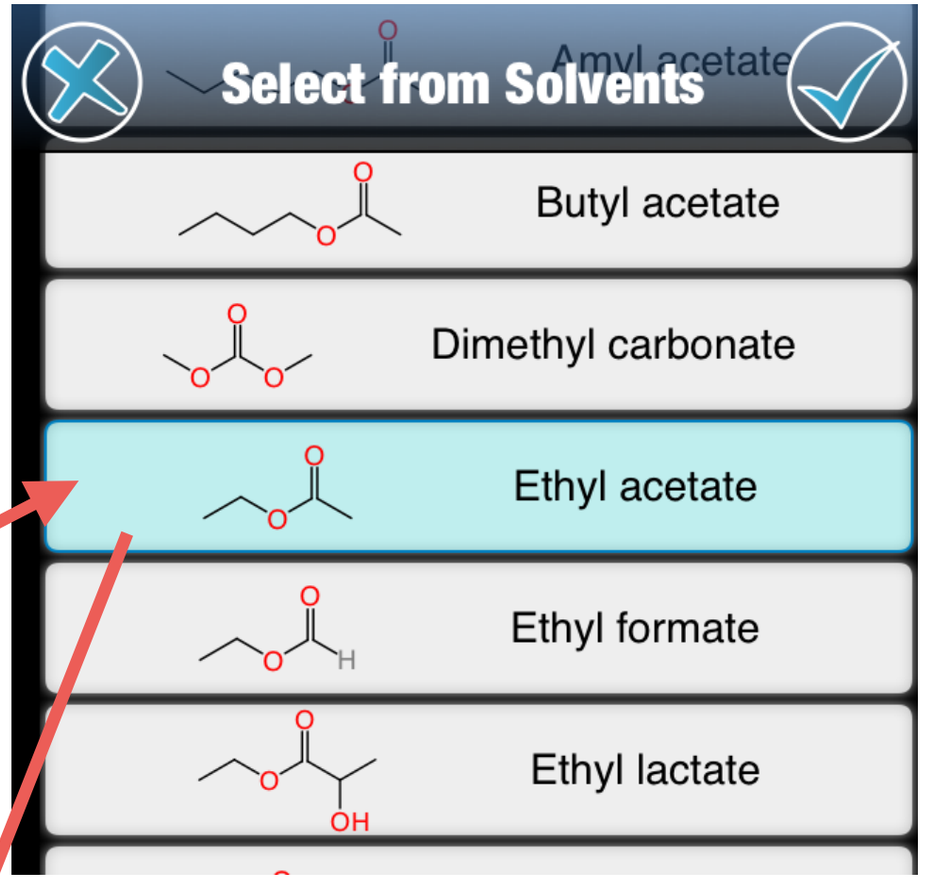
Waste disposal

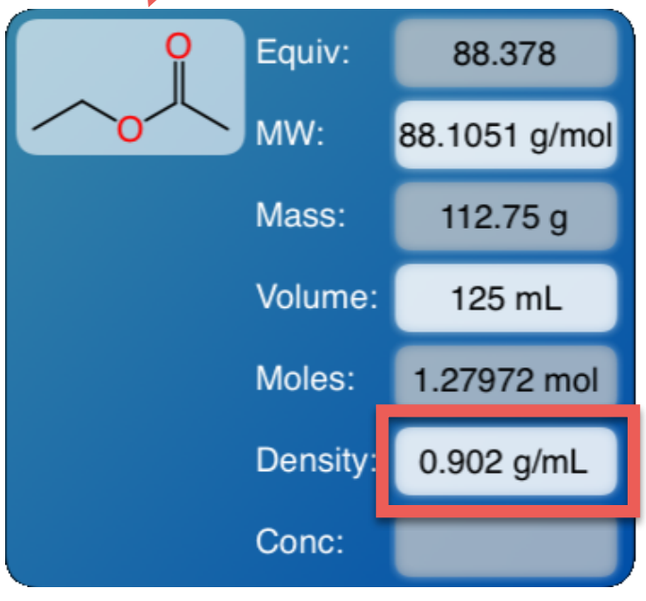
Reactivity

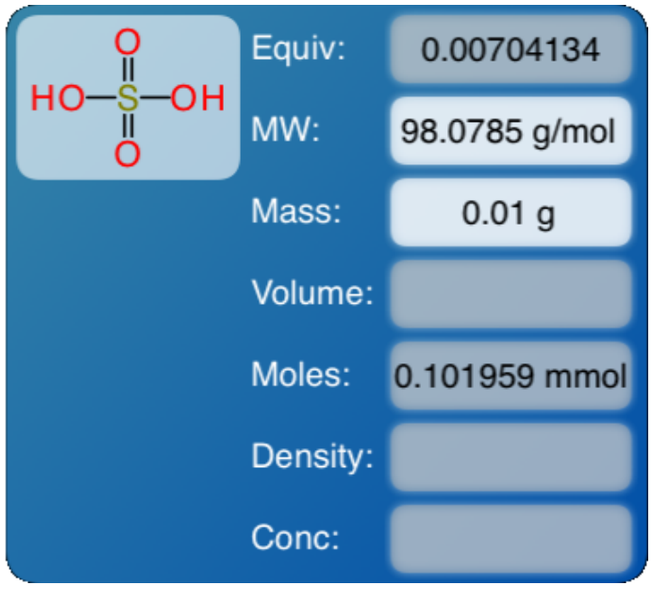
Lifecycle

Using Solvents

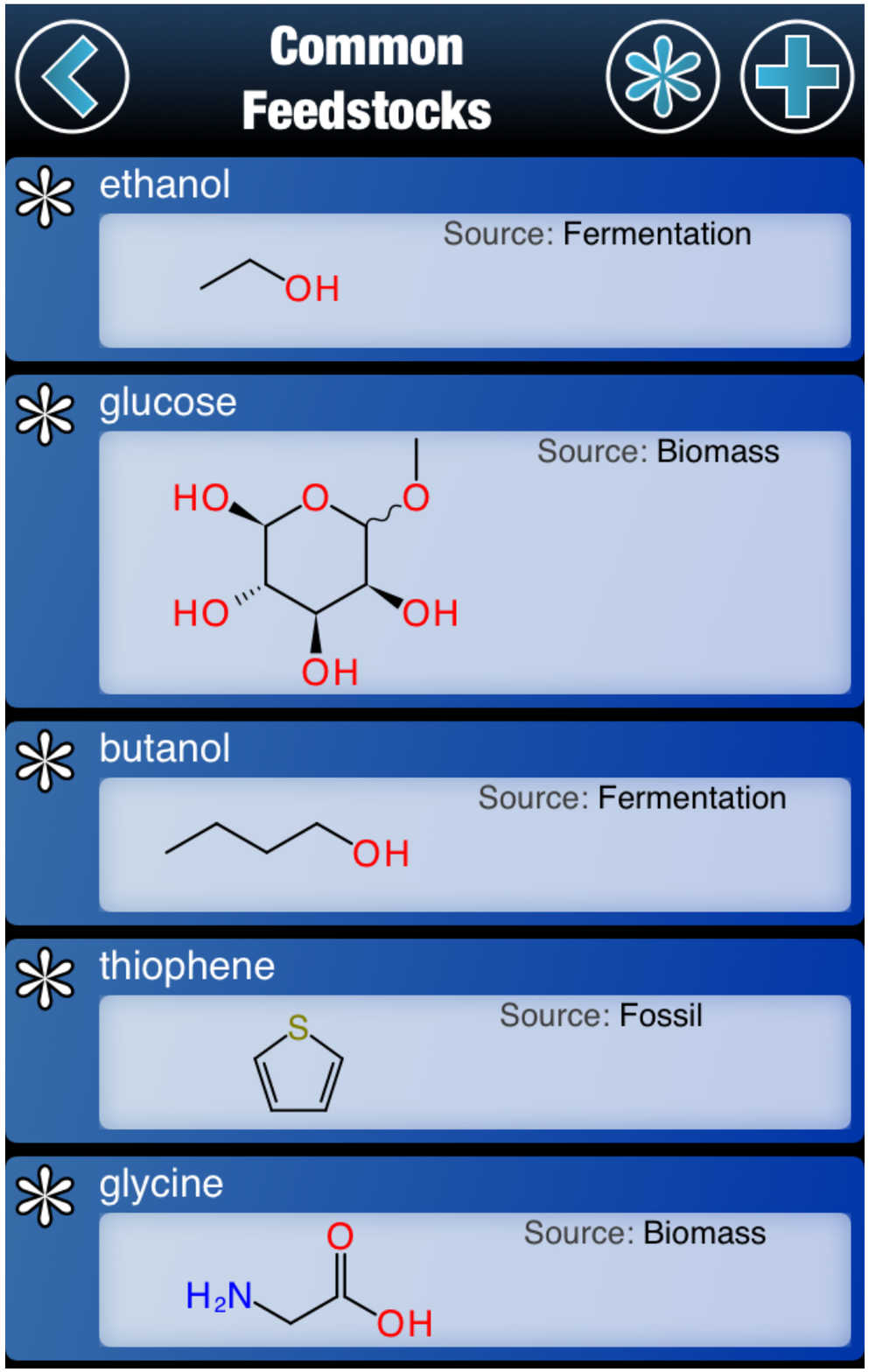






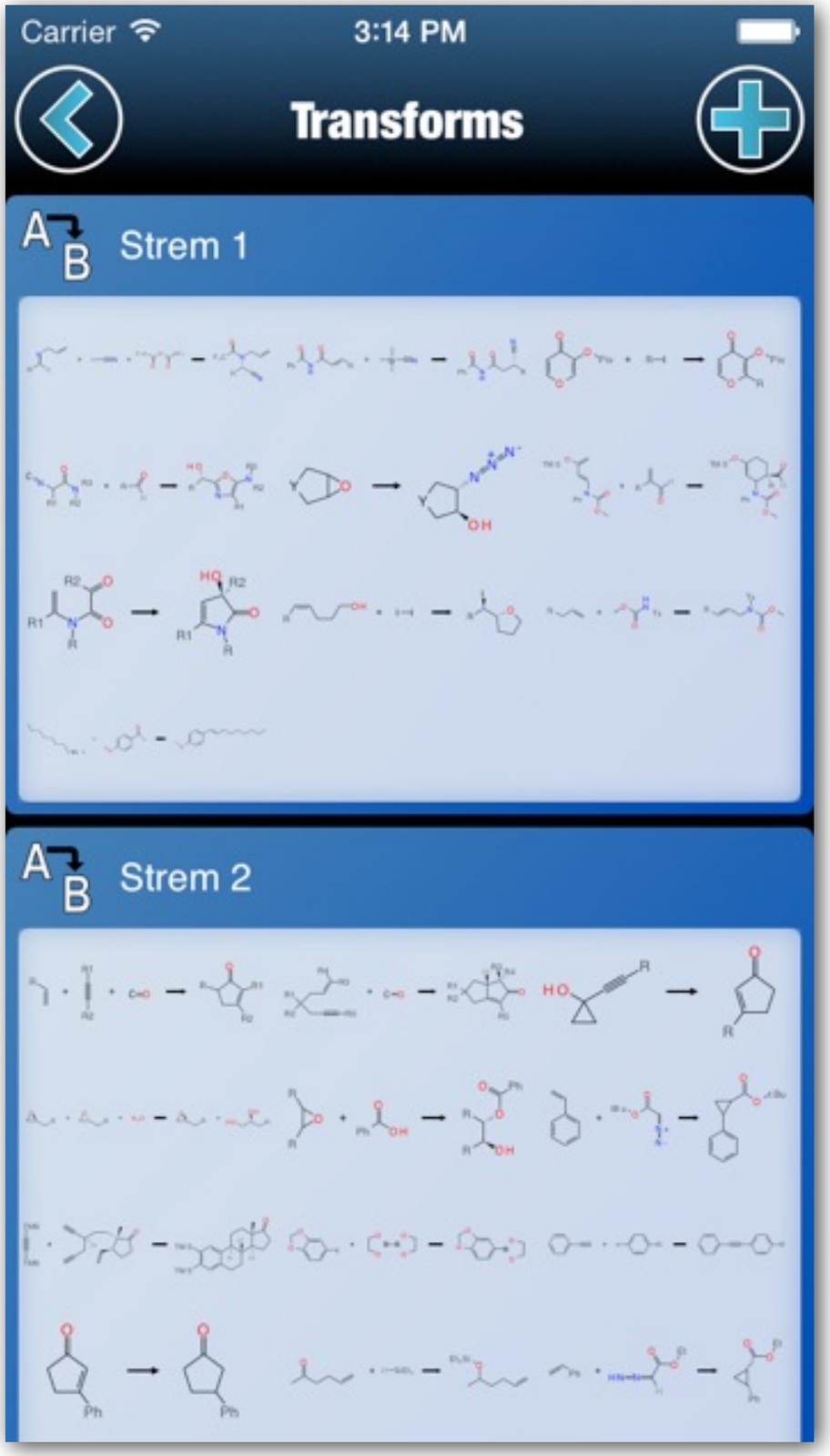


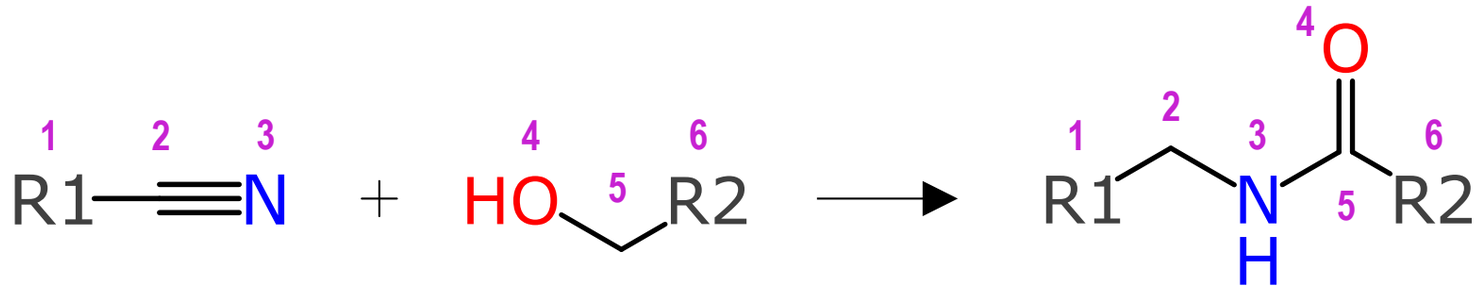
Feedstocks



- Not all starting materials are created equal
- Some can be made from renewable sources
- Lab notebook is a chance to guide & educate
- Curation is a work in progress…

Transforms





- Chemical reactions can be curated as *transforms*
- Can be used to search for ways to design a reaction
- Curation of **green transforms** is a way to encourage preferred reaction pathways

Availability

- The **Green Lab Notebook** (GLN) app should be in the iTunes AppStore by autumn

- For iPhones, iPods & iPads

- In the meanwhile, check out:

Green Solvents

Reaction101

Lab Solvents

Yield101

Acknowledgments

- Sean Ekins (Green Solvents)
- Inquiries to **info@molmatinf.com**

MOLECULAR MATERIALS INFORMATICS

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